Chapter 2. Quantum Dynamics (in closed systems)

2.1 Time evolution and Schrödinger equation

In Chapter 1, we had "spatial" translation. ($\hat{x}$)

Now, we need "time" to describe "dynamics".

(1) Time-Evolution Operator. $\mathcal{U}(t, t_0)$

- notation : $|\alpha, t_0; t\rangle = \mathcal{U}(t, t_0)\, |\alpha, t_0\rangle$

State at t, used to be $|\alpha\rangle$ at t_0

Time-Evolution op. of $t_0 \to t$

state ket $|\alpha\rangle$ prepared at time "t".

- property of the time-evolution operator

① It's a unitary operator.

$$\mathcal{U}^\dagger(t, t_0)\, \mathcal{U}(t, t_0) = \mathbb{1} \quad (\text{also, } \mathcal{U}\mathcal{U}^\dagger = I)$$

$\Rightarrow$ Time-evolution does not change the sum of probabilities $= 1$.

: norm is always 1.

$$\langle \alpha, t_0; t | \alpha, t_0; t\rangle = \langle \alpha, t_0 |\, \mathcal{U}^\dagger(t, t_0)\, \mathcal{U}(t, t_0)\, |\alpha, t_0\rangle$$

$$= 1.$$

(Right-to-Left!)

② $\mathcal{U}(t_2, t_0) = \mathcal{U}(t_2, t_1)\, \mathcal{U}(t_1, t_0)$

: successive time-evolution.

$$t_0 \xrightarrow{\ \mathcal{U}\ } t_1 \xrightarrow{\ \mathcal{U}\ } t_2$$

$$= \quad t_0 \xrightarrow[\ \mathcal{U}\ ]{} t_2$$

Note : physically, $t_2 > t_1 > t_0$,

but "effective" backward evolution is also possible.

- So, what does $\mathcal{U}(t, t_0)$ look like?

$\Leftarrow$ It's just like "time"-version of the translation operator "$\mathcal{J}$".

previously, it was $x \to x + \delta x$,

now, it is $t_0 \to t_0 + \delta t$!

$\Rightarrow$ infinitesimal t-evolution operator

$$\mathcal{U}(t_0 + \delta t, t_0) = 1 - i\tilde{\Omega}\delta t$$

$\mathcal{J}(\delta x) = 1 - i\tilde{K}\delta x$: spatial translation

- $\tilde{\Omega}$: a Hermitian operator ($\tilde{\Omega}^{\dagger} = \tilde{\Omega}$) $\leftrightarrow$ ($\tilde{K}^{\dagger} = \tilde{K}$)

(because of $\mathcal{U}^{\dagger}\mathcal{U} = 1$)

- check if the properties of $\mathcal{U}$ are valid with this form.

- Now, what does "$\tilde{\Omega}$" look like?

previously, in spatial translation,

$\tilde{K} = \tilde{P}/\hbar$ $\Leftarrow$ classical-quantum correspondence

: momentum is a generator of linear translation.

$\hookrightarrow$ What is a generator of "time" translation in classical Mechanics?

$\Rightarrow$ Hamiltonian.

Thus, $$\boxed{\tilde{\Omega} = \frac{\tilde{H}}{\hbar}}$$

: unit $= [T]^{-1}$

$[H] = [E] = [\hbar\omega]$

where $[\omega] = [T]^{-1}$.

- But, there is a "Big"(?) difference between spatial and time translations.

$$\mathcal{J}(\delta x) = 1 - i\frac{\tilde{P}}{\hbar}\delta x \longleftrightarrow \mathcal{U}(\delta t) = 1 - i\frac{\tilde{H}}{\hbar}\delta t$$

$\uparrow$ x is an "operator". $\uparrow$ t is a "parameter".

- What happens if "t" is an operator?

(it's fair in terms of special relativity).

from $\mathcal{J}$

$$\Rightarrow [\tilde{x}_i, \tilde{P}_i] = i\hbar\delta_{ij} \longrightarrow [\tilde{t}, \tilde{H}] = i\hbar$$

meaning of $[\tilde{t}, \tilde{H}] = i\hbar$: (infinite uncertainty as $\Delta t \to 0$)

There is no bound in Energy!

: unphysical. $\rightarrow$ $\boxed{t \text{ cannot be an operator!}}$

- What we're doing here ; "Canonical Quantization".

$\rightarrow$ $\tilde{x}$ is an operator ; t is a parameter

c.f. Quantum field Theory (+second quantization)

$\rightarrow$ "field" is an operator

; (x, y, z, t) is a parameter of the field.

(2) Schrödinger Equation

→ differential eq. for $\mathcal{U}$

infinitesimal

try $\mathcal{U}(t+\delta t, t_0) = \mathcal{U}(t+\delta t, t)\,\mathcal{U}(t, t_0)$

$$= \left(1 - i\frac{H}{\hbar}\delta t\right)\mathcal{U}(t, t_0)$$

$$\Rightarrow \quad \frac{\mathcal{U}(t+\delta t, t_0) - \mathcal{U}(t, t_0)}{\delta t} = -i\frac{H}{\hbar}\,\mathcal{U}(t, t_0)$$

as $\delta t \to 0$

$$\Rightarrow \quad \boxed{i\hbar\frac{\partial}{\partial t}\mathcal{U}(t, t_0) = H\,\mathcal{U}(t, t_0)}$$

Schrödinger eq. for $\mathcal{U}$.

- For a state ket $|\alpha\rangle$, (prepared at t_0)

$$i\hbar\frac{\partial}{\partial t}\mathcal{U}(t, t_0)|\alpha, t_0\rangle = H\,\mathcal{U}(t, t_0)|\alpha, t_0\rangle$$

$$\Rightarrow \quad \boxed{i\hbar\frac{\partial}{\partial t}|\alpha, t_0; t\rangle = H|\alpha, t_0; t\rangle}$$

This is the Schrödinger eq. that we know.

* Explicit form of $\mathcal{U}(t, t_0)$.

<u>Case 1.</u> H = time-independent.

Solve!

$$i\hbar\frac{\partial}{\partial t}\mathcal{U}(t, t_0) = H\,\mathcal{U}(t, t_0) \Rightarrow \underline{\mathcal{U}(t, t_0) = e^{-\frac{i}{\hbar}H(t-t_0)}}$$

infinite-steps of infinitesimal t-evolutions

or) $$\lim_{N\to\infty}\left[1 - \frac{i}{\hbar}H\left(\frac{t-t_0}{N}\right)\right]^N = \exp\left[-\frac{i}{\hbar}H(t-t_0)\right]$$

verification

$$\exp\left[-\frac{i}{\hbar}H(t-t_0)\right] = 1 - \frac{i}{\hbar}H(t-t_0) + \frac{1}{2!}\cdot\frac{(-i)^2}{\hbar^2}H^2(t-t_0)^2 + \cdots$$

$$\frac{d}{dt}[\ \checkmark\ ] = -\frac{i}{\hbar}H + \frac{1}{2}\cdot\left(\frac{-i}{\hbar}\right)^2 H^2\cdot 2(t-t_0) + \cdots$$

$$= -\frac{i}{\hbar}H\left(\underbrace{1 - \frac{i}{\hbar}H(t-t_0) + \cdots}\right)$$

$$= U(t-t_0)$$

Case 2. H : time-dependent, but $[H(t_1), H(t_2)] = 0$ //.

$$\Rightarrow U(t,t_0) = \exp\left[-\frac{i}{\hbar}\int_{t_0}^{t} dt' H(t')\right]$$

case 3. $[H(t_1), H(t_2)] \neq 0$.

ex. spin-$\frac{1}{2}$ in a magnetic field

$H \propto \vec{S}\cdot\vec{B}(t)$ → if $\vec{B}(t) = B(t)\hat{z}$ (same dir.)

$\Rightarrow [H(t_1), H(t_2)] = 0$.

→ if $\vec{B}(t) = B_x(t)\hat{x} + B_y(t)\hat{y}$

$\Rightarrow [H(t_1), H(t_2)] \neq 0$

$$\Rightarrow U(t,t_0) = \text{"}T\text{"} \exp\left[-\frac{i}{\hbar}\int_{t_0}^{t} dt' H(t')\right].$$

↑ time-ordering operator.

expansion :

$$\Rightarrow U(t,t_0) = 1 + \left(\frac{-i}{\hbar}\right)\int_{t_0}^{t} dt_1 H(t_1)$$

$$+ \left(\frac{-i}{\hbar}\right)^2 \int_{t_0}^{t} dt_1 \int_{t_0}^{t_1} dt_2\, H(t_1)H(t_2)$$

$$+ \left(\frac{-i}{\hbar}\right)^3 \int_{t_0}^{t} dt_1 \int_{t_0}^{t_1} dt_2 \int_{t_0}^{t_2} dt_3\, \underbrace{H(t_1)H(t_2)H(t_3)}_{\text{time-ordered!}}$$

$$+ \cdots$$

* meaning of the "time-ordering" operator

Let's try to find a solution iteratively.

Try $U^{(0)}=1 \longrightarrow i\hbar\frac{\partial}{\partial t'}U^{(1)} = H(t') \to U = 1 + \frac{1}{i\hbar}\int_{t_0}^{t} dt'\, H(t')$

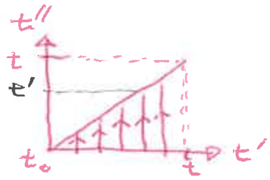
$$U^{(1)}(t,t_0) = 1 + \frac{1}{i\hbar}\int_{t_0}^{t} dt'\, H(t') \Rightarrow i\hbar\frac{d}{dt'}U^{(2)} = H(t') + H(t')\frac{1}{i\hbar}\int_{t_0}^{t'} dt''\, H(t')$$

$$\to U^{(2)}(t,t_0) = 1 + \frac{1}{i\hbar}\int_{t_0}^{t} dt'\, H(t') + \left(\frac{1}{i\hbar}\right)^2 \int_{t_0}^{t} dt'\, H(t') \int_{t_0}^{t'} dt''\, H(t')$$

$$U^{(2)}(t,t_0) \to U^{(3)}(t,t_0) \to \cdots$$

$$\Rightarrow U(t,t_0) = 1 + \sum_{n=1}^{\infty}\left(\frac{1}{i\hbar}\right)^n \int_{t_0}^{t} dt_1 \int_{t_0}^{t_1} dt_2 \cdots \int_{t_0}^{t_{n-1}} dt_n\, H(t_1)H(t_2)\cdots H(t_n)$$

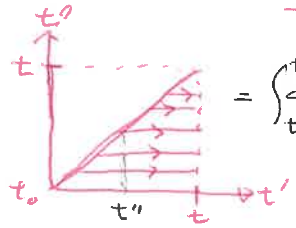
No $\boxed{n!}$ factor! (Dyson series)



• Second order term :

$$\int_{t_0}^{t} dt' \int_{t}^{t'} dt''\, H(t')H(t'') = \left[\frac{1}{2}\int_{t_0}^{t} dt' \int_{t_0}^{t'} dt''\, H(t')H(t'')\right]$$

$$+ \left[\frac{1}{2}\int_{t_0}^{t} dt' \int_{t'}^{t} dt''\, H(t'')H(t')\right] \quad t' \leftrightarrow t''$$



$$= \int_{t_0}^{t} dt'' \int_{t''}^{t} dt'\, H(t')H(t'')$$

$$= \frac{1}{2!}\int_{t_0}^{t} dt' \int_{t_0}^{t} dt''\, \mathrm{T}\left[H(t')H(t'')\right]$$

def. time-ordering op.

where $\mathrm{T}[A(t')B(t'')] = \Theta(t'-t'')\, A(t')B(t'') + \Theta(t''-t')\, B(t'')A(t')$

$$\Rightarrow U(t,t_0) = \mathrm{T}\exp\left[-\frac{i}{\hbar}\int_{t_0}^{t} dt'\, H(t')\right]$$

(3) Energy eigenkets.

If we know the eigenkets of H : $\{|n\rangle, E_n\}$.

$$\Rightarrow \quad H|n\rangle = E_n|n\rangle$$

can be a collective index. of $(a, b, c, d \cdots)$, given by

a complete set of mutually commuting observables

$$[A, B] = [B, C] = \cdots = 0$$

$$[H, A] = [H, B] = \cdots = 0.$$

- representation of $U(t) = \exp[-\frac{iHt}{\hbar}]$ || $t_0 = 0$. H : t-indep.

$$\Rightarrow U(t) = \sum_{n', n''} |n''\rangle\langle n''| e^{-\frac{iHt}{\hbar}} |n'\rangle\langle n'|$$

$$= \sum_{n'} |n'\rangle e^{-\frac{iE_{n'}t}{\hbar}} \langle n'|.$$

- time-evolution of a state ket $(t_0 = 0)$

$$|\alpha\rangle = \sum_n |n\rangle\langle n|\alpha\rangle = \sum_n c_n |n\rangle$$

$$|\alpha; t\rangle = e^{-\frac{iHt}{\hbar}} |\alpha\rangle = \sum_n e^{-\frac{iHt}{\hbar}} |n\rangle\langle n|\alpha\rangle$$

$$= \sum_n \underbrace{c_n e^{-\frac{iE_nt}{\hbar}}}_{\equiv\, c_n(t)} |n\rangle$$

(4) Time dependence of Expectation values.

① Stationary state.

$|\alpha\rangle = |n\rangle$: measured at an eigenstate.

c-number!

$$\langle\alpha;t|B|\alpha;t\rangle = \langle\alpha| U^{\dagger}(t)\, B\, U(t) |\alpha\rangle$$

$$= \langle n| \cancel{\exp(\frac{iE_nt}{\hbar})} \cdot B\, \cancel{\exp(-\frac{iE_nt}{\hbar})} |n\rangle$$

$$= \langle n|B|n\rangle \; : \; t\text{-independent!}$$

② non-stationary state

$$|\alpha\rangle = \sum_n c_n |n\rangle \quad \left(\text{not in a particular eigenstate !}\right).$$

$$\langle \alpha; t | B | \alpha; t\rangle = \sum_{n'} c_{n'}^* \langle n' | e^{\frac{iE_{n'}t}{\hbar}} \cdot B \cdot \sum_{n''} c_{n''} e^{-\frac{iE_{n''}t}{\hbar}} |n''\rangle$$

$$= \sum_{n', n''} c_{n'}^* c_{n''} \langle n' | B | n''\rangle e^{-i\omega_{n''n'}t}$$

where $\omega_{n''n'} = \dfrac{E_{n''} - E_{n'}}{\hbar}$

$\Rightarrow$ oscillations !!

(5) example : spin precession. (spin-$\frac{1}{2}$ system).

- $H = -\alpha \underset{\sim}{\vec{S}} \cdot \vec{B}$, $\alpha = \dfrac{e}{m_e c}$, $\vec{B} = B\hat{z}$ (uniform B-field)

$$= -\left(\frac{eB}{m_e c}\right) \tilde{S}_z \quad (e<0 \text{ for electrons}).$$

eigenstates : $E_\pm = \mp \dfrac{e\hbar B}{2m_e c}$ for $|\pm\rangle$.

$\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad |||$

$\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad |\uparrow\rangle, |\downarrow\rangle$ in our notation.

letting $\omega \equiv \dfrac{|e|B}{m_e c}$, $H \equiv \omega \tilde{S}_z$

- time-evolution operator

$$U(t) = \exp\left[\frac{-i\omega \tilde{S}_z t}{\hbar}\right].$$

- time-evolution from a state ket $|\alpha\rangle$

$$|\alpha\rangle = C_+ |\uparrow\rangle + C_- |\downarrow\rangle$$

$$\rightarrow |\alpha;t\rangle = C_+ e^{-\frac{i\omega t}{2}} |\uparrow\rangle + C_- e^{\frac{i\omega t}{2}} |\downarrow\rangle$$

$$\Big\| \quad H|\uparrow\rangle = \frac{\hbar\omega}{2}|\uparrow\rangle, \quad H|\downarrow\rangle = -\frac{\hbar\omega}{2}|\downarrow\rangle.$$

- example: $|\alpha\rangle = |\uparrow\rangle$, ~~it~~ an eigen ket.

  No t-dependence.

- example: $|\alpha\rangle = |S_x;+\rangle = \frac{1}{\sqrt{2}}|\uparrow\rangle + \frac{1}{\sqrt{2}}|\downarrow\rangle$.

$\Rightarrow$ Prob. ~~of~~ finding $|S_x;\pm\rangle$ state at time t:

$$\left|\langle S_x;\pm|\alpha;t\rangle\right|^2 = \left| \left[\frac{1}{\sqrt{2}}\langle\uparrow| \pm \frac{1}{\sqrt{2}}\langle\downarrow|\right] \cdot \left[\frac{1}{\sqrt{2}} e^{-\frac{i\omega t}{2}}|\uparrow\rangle + \frac{1}{\sqrt{2}} e^{\frac{i\omega t}{2}}|\downarrow\rangle\right]\right|^2$$

$$= \left|\frac{1}{2} e^{-\frac{i\omega t}{2}} \pm \frac{1}{2} e^{\frac{i\omega t}{2}}\right|^2$$

$$= \begin{cases} \cos^2\frac{\omega t}{2} & \text{for } |S_x;+\rangle \\ \sin^2\frac{\omega t}{2} & \text{for } |S_x;-\rangle \end{cases}$$

$\Rightarrow$ observables.

$$\langle \tilde{S}_x\rangle \equiv \langle\alpha;t|\tilde{S}_x|\alpha;t\rangle = \frac{\hbar}{2}\cos\omega t$$

($\tilde{S}_x = \frac{\hbar}{2}\left[|\uparrow\rangle\langle\downarrow| + |\downarrow\rangle\langle\uparrow|\right]$)

$$\langle\tilde{S}_y\rangle = \frac{\hbar}{2}\sin\omega t$$

$$\langle\tilde{S}_z\rangle = 0.$$